

Table S1. Non-bonded distances in the active site of mature PG

Atom	Atom	Distance (Å)	Estimated deviation (Å)
Cys156 S γ	Na	2.17	0.17
Cys156 S γ	His197N δ 1	3.82	0.05
Cys156 S γ	Tyr196O η	3.87	0.07
Cys156 S γ	W1	3.06	0.07
Cys156 N	Na	2.89	0.16
His197N δ 1	W1	2.88	0.06
His197N ε 2	Asp217O δ 2	2.76	0.06
Asp217O δ 2	Trp231N ε	2.88	0.04
Asp217O δ 1	Ser219O γ A	2.67	0.03
Asp217O δ 1	W3	2.77	0.03
Arg159N ε	W3	2.85	0.04
Arg159N ε	Ser219O γ A	2.84	0.04
Arg159N η 1	W2	2.69	0.04
Arg159N η 2	W2	2.80	0.04
W1	W2	2.92	0.06
W1	Na	2.50	0.18